Mel Levy

List of Publications by Year
in descending order

78 papers	13,402 citations	136885 32 h-index	79644 73 g-index
80 all docs	80 docs citations	80 times ranked	6591 citing authors

#	Article	IF	Citations
1	Electronegativity: The density functional viewpoint. Journal of Chemical Physics, 1978, 68, 3801-3807.	1.2	2,806
2	Density-Functional Theory for Fractional Particle Number: Derivative Discontinuities of the Energy. Physical Review Letters, 1982, 49, 1691-1694.	2.9	2,573
3	Physical Content of the Exact Kohn-Sham Orbital Energies: Band Gaps and Derivative Discontinuities. Physical Review Letters, 1983, 51, 1884-1887.	2.9	2,105
4	Hellmann-Feynman, virial, and scaling requisites for the exact universal density functionals. Shape of the correlation potential and diamagnetic susceptibility for atoms. Physical Review A, 1985, 32, 2010-2021.	1.0	897
5	Exact differential equation for the density and ionization energy of a many-particle system. Physical Review A, 1984, 30, 2745-2748.	1.0	803
6	Electron densities in search of Hamiltonians. Physical Review A, 1982, 26, 1200-1208.	1.0	570
7	Exact Kohn-Sham scheme based on perturbation theory. Physical Review A, 1994, 50, 196-204.	1.0	506
8	Perspective on "Density functional approach to the frontier-electron theory of chemical reactivity". Theoretical Chemistry Accounts, 2000, 103, 353-360.	0.5	424
9	Correlation-energy functional and its high-density limit obtained from a coupling-constant perturbation expansion. Physical Review B, 1993, 47, 13105-13113.	1.1	385
10	Density-functional exchange correlation through coordinate scaling in adiabatic connection and correlation hole. Physical Review A, 1991, 43, 4637-4646.	1.0	261
11	Variational Density-Functional Theory for an Individual Excited State. Physical Review Letters, 1999, 83, 4361-4364.	2.9	180
12	Strictly correlated electrons in density-functional theory. Physical Review A, 1999, 59, 51-54.	1.0	146
13	DFT ionization formulas and aDFT perturbation theory for exchange and correlation, through adiabatic connection. International Journal of Quantum Chemistry, 1995, 56, 93-108.	1.0	142
14	Correlation-energy density-functional formulas from correlating first-order density matrices. Physical Review A, 1995, 52, R1808-R1810.	1.0	98
15	Hybrid schemes combining the Hartree–Fock method and density-functional theory: Underlying formalism and properties of correlation functionals. Journal of Chemical Physics, 1997, 106, 2675-2680.	1.2	97
16	Generalized density-functional theory: Conquering theN-representability problem with exact functionals for the electron pair density and the second-order reduced density matrix. Journal of Chemical Sciences, 2005, 117, 507-514.	0.7	79
17	Relation between exchange-only optimized potential and Kohn–Sham methods with finite basis sets, and effect of linearly dependent products of orbital basis functions. Journal of Chemical Physics, 2008, 128, 104104.	1.2	61
18	Density functionals for exchange and correlation energies: Exact conditions and comparison of approximations. International Journal of Quantum Chemistry, 1994, 49, 539-548.	1.0	60

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19	Exact high-density limit of correlation potential for two-electron density. Journal of Chemical Physics, 1999, 110, 10262-10268.	1.2	54
20	Approximate noninteracting kinetic energy functionals from a nonuniform scaling requirement. International Journal of Quantum Chemistry, 1991, 40, 379-388.	1.0	53
21	Time-independent density-functional theory for excited states of Coulomb systems. Physical Review A, 2012, 85, .	1.0	53
22	Direct first principles algorithm for the universal electron density functional. Journal of Chemical Physics, 1982, 77, 396-398.	1.2	52
23	Line-integral formulas for exchange and correlation potentials separately. Physical Review A, 1997, 55, 1885-1889.	1.0	47
24	A new functional with homogeneous coordinate scaling in density functional theory: Fâ€‰[â€‰Ï¡Î»]. Journal of Chemical Physics, 1985, 83, 2334-2336.	1.2	46
25	Expectation values in density-functional theory, and kinetic contribution to the exchange-correlation energy. Physical Review B, 1993, 47, 1167-1173.	1.1	45
26	Time-independent (static) density-functional theories for pure excited states: Extensions and unification. Physical Review A, 2009, 80, .	1.0	44
27	Density-functional exchange identity from coordinate scaling. Physical Review A, 1996, 53, 3140-3142.	1.0	42
28	An energyâ€“density equation for isoelectronic changes in atoms. Journal of Chemical Physics, 1978, 68, 5298-5299.	1.2	40
29	Sum rules for exchange and correlation potentials. Journal of Chemical Physics, 2001, 115, 4438-4443.	1.2	39
30	Ground-State Energy as a Simple Sum of Orbital Energies in Kohn-Sham Theory: A Shift in Perspective through a Shift in Potential. Physical Review Letters, 2014, 113, 113002.	2.9	39
31	Atomic binding energies from fundamental theorems involving the electron density, â€˜râˆ�’1ã€‰, and the Zâˆ’1 perturbation expansion. Journal of Chemical Physics, 1980, 72, 3416-3417.	1.2	37
32	Rigorous and approximate relations between expectation values of atoms. Journal of Chemical Physics, 1980, 72, 4009-4013.	1.2	37
33	Average Local Ionization Energies in the Hartreeâˆ’Fock and Kohnâˆ’Sham Theories. Journal of Physical Chemistry A, 2009, 113, 1384-1389.	1.1	32
34	Success of quantum mechanical approximations for molecular geometries and electronâ€"nuclear attraction expectation values: Gift of the Coulomb potential?. Journal of Chemical Physics, 1986, 84, 4519-4523.	1.2	30
35	Electron density-functional theory and x-ray structure factors. Physical Review B, 1987, 35, 7887-7890.	1.1	30
36	Recent constrained-search advances for approximating density functionals. The Philosophical Magazine: Physics of Condensed Matter B, Statistical Mechanics, Electronic, Optical and Magnetic Properties, 1994, 69, 763-769.	0.6	30

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37	A discontinuous energy–density functional. Journal of Chemical Physics, 1982, 77, 3140-3147.	1.2	28
38	Connections between ground-state energies from optimized-effective potential exchange-only and Hartree–Fock methods. Journal of Chemical Physics, 2003, 119, 7087-7093.	1.2	26
39	Method for direct determination of localized orbitals. Journal of Chemical Physics, 1975, 63, 316-318.	1.2	24
40	Accurate correlation potentials from integral formulation of density functional perturbation theory. Journal of Chemical Physics, 2002, 116, 6924-6929.	1.2	24
41	On approximate energy differences from average electron densities. Journal of Chemical Physics, 1979, 70, 1573-1574.	1.2	23
42	On the simple constrained–search reformulation of the Hohenberg–Kohn theorem to include degeneracies and more (1964–1979). International Journal of Quantum Chemistry, 2010, 110, 3140-3144.	1.0	23
43	Energy–density relations and screening constants in atoms. Journal of Chemical Physics, 1980, 73, 5168-5173.	1.2	22
44	Improving energies by using exact electron densities. Physical Review A, 1996, 53, R2915-R2917.	1.0	22
45	Augmented potential, energy densities, and virial relations in the weak- and strong-interaction limits of DFT. Journal of Chemical Physics, 2017, 147, 214107.	1.2	22
46	Connections between High-Density Scaling Limits of DFT Correlation Energies and Second-Order Z^{-1} Quantum Chemistry Correlation Energy. Journal of Physical Chemistry A, 1998, 102, 3151-3156.	1.1	20
47	Comment on "Functional derivative of the universal density functional in Fock space". Physical Review A, 2009, 79, .	1.0	17
48	Asymptotic coordinate scaling bound for exchange-correlation energy in density-functional theory. International Journal of Quantum Chemistry, 1989, 36, 617-619.	1.0	17
49	Bounds for the exchange and correlation potentials. Physical Review A, 1995, 51, 2851-2856.	1.0	15
50	Mathematical thoughts in DFT. International Journal of Quantum Chemistry, 2016, 116, 802-804.	1.0	12
51	Unconstrained exchange localization and distant orbital tails. Journal of Chemical Physics, 1976, 65, 2473-2475.	1.2	11
52	The nearest self–adjoint operator. Journal of Chemical Physics, 1980, 72, 780-781.	1.2	11
53	Kinetic energy from a single Kohn-Sham orbital. Physical Review A, 2009, 79, .	1.0	11
54	Energy differences from electrostatic potentials at nuclei. Journal of Chemical Physics, 1987, 87, 5044-5046.	1.2	10

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55	Approach to density-functional ionization energy. Physical Review B, 1996, 53, 969-972.	1.1	10
56	Formal expressions and corresponding expansions for the exact Kohn-Sham exchange potential. Physical Review A, 2009, 80, .	1.0	10
57	Kinetic and electron-electron energies for convex sums of ground state densities with degeneracies and fractional electron number. Journal of Chemical Physics, 2014, 140, 18A538.	1.2	10
58	Simple hydrogenic estimates for the exchange and correlation energies of atoms and atomic ions, with implications for density functional theory. Journal of Chemical Physics, 2020, 153, 074114.	1.2	10
59	Exact local exchange potential from Fock equations at vanishing coupling constant, and $Îc/Î´n$ from wave-function calculations at full coupling constant. Physical Review A, 1996, 53, 3963-3965.	1.0	9
60	New exact relations for improving the exchange and correlation potentials. International Journal of Quantum Chemistry, 1995, 56, 385-388.	1.0	8
61	Closed-form expression relating the second-order component of the density functional theory correlation energy to its functional derivative. Journal of Chemical Physics, 1998, 109, 6280-6286.	1.2	8
62	Nodal variational principle for excited states. Physical Review A, 2018, 98, .	1.0	8
63	Highly Excited States from a Time Independent Density Functional Method. Computation, 2016, 4, 28.	1.0	7
64	Variational energy functionals involving one–electron operators. Journal of Chemical Physics, 1977, 67, 724-726.	1.2	6
65	Adiabatic integration formula for the correlation energy functional of the Hartree-Fock density. Theoretical Chemistry Accounts, 1999, 103, 117-123.	0.5	6
66	Tight constraints on the exchange-correlation potentials of degenerate states. Journal of Chemical Physics, 2014, 140, 18A537.	1.2	6
67	On augmented Kohn–Sham potential for energy as a simple sum of orbital energies. Molecular Physics, 2016, 114, 1162-1164.	0.8	6
68	Approximating the Shifted Hartree-Exchange-Correlation Potential in Direct Energy Kohn–Sham Theory. Journal of Chemical Theory and Computation, 2018, 14, 684-692.	2.3	6
69	Additive density functional correlation corrections to single particle theories. International Journal of Quantum Chemistry, 1997, 61, 281-285.	1.0	3
70	Properties of Augmented Kohn–Sham Potential for Energy as Simple Sum of Orbital Energies. Journal of Physical Chemistry A, 2017, 121, 342-347.	1.1	3
71	Density- and spin-density-functional theories through spin-free wave functions. Physical Review A, 2019, 100, .	1.0	3
72	On the best partitioning of the density functional energy. Journal of Molecular Modeling, 2018, 24, 311.	0.8	1

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73	THEOREMS FOR EXACT LOCAL EXCHANGE POTENTIAL. Modern Physics Letters B, 1991, 05, 1613-1616.	1.0	0
74	Pointwise and generalized virial theorems. International Journal of Quantum Chemistry, 1978, 14, 343-344.	1.0	0
75	Properties of the exact universal density and one-matrix functionals. International Journal of Quantum Chemistry, 1985, 28, 743-744.	1.0	0
76	Energy components in spin-density functional theory. Physical Review A, 2021, 104, .	1.0	0
77	Line-integral formulas for exchange and correlation potentials separately. World Scientific Series in 20th Century Physics, 2009, , 613-617.	0.0	0
78	On the adiabatic connection method, and scaling of electron–electron interactions in the Thomas–Fermi limit. World Scientific Series in 20th Century Physics, 2009, , 542-545.	0.0	0